Simulation of transverse electron transport in resonant tunneling diode

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***Abstract**: Fast and stable stationary numerical model of electronic transport in resonant-tunneling diode (RTD) was developed. It was derived from the density functional method, applying assumption about the absence of exchange-correlation term. The model correctly describes interaction between quantum and semi-classical regions of RTD. Self-consistence between space charge and potential can be achieved for all relevant RTD structures. The results of modeling were tested for the model structures of RTDs with barrier layers formed of $Al_xGa_{1-x}As$ and $Al_xGa_{1-x}N$. There is a possibility of efficient visualization of modeling results, such as local density of states, potential and electron concentration in active region.*

1. INTRODUCTION

The modeling of resonant-tunneling diodes has passed several stages since its invention. The formalisms of wave functions [1], Green's and Wigner's functions [2,3] were used by different authors since pioneering work [4] by present time. The way of improving consists in the procedure of self-consistency, accurate consideration of band structure of the corresponding materials and taking scattering processes into account [5]. Successive application of all mentioned components leads to enormous complications of numerical modeling procedure. Under such conditions appropriate numerical methods have to be used. Two main demands for numerical methods used in a given work was made: correct formulating of numerical algorithms taking physical processes that expect to take place in the device into account (1), and choosing as fast numerical method as possible under the stipulation that it will reflect the actual physical picture (2).

2. ASSUMPTIONS

The most fundamental assumptions made in the developed model are as follows.

The model is quasi-one-dimensional. The only charge carriers to be considered are electrons in conduction band. In the active region of the structure electrons considered to be quasi-particles when they move along the planes of heterostructure's layers. At the same time, electrons considered to be quantum particles at the active region and characterized by wave functions, depending on the fields, in which electrons move. The whole nanostructure divides into 3 regions: left and right reservoirs and active region corresponding to fig. 1. Electron's collective at the left and right reservoirs considered to be at local equilibrium, each with one's Fermi level, E_F^L and E_F^R consequently, while electron gas at the active region is far from equilibrium and cannot be characterized by means of even modified Fermi-Dirac statistics.

Our goal is to find electron transmission function $T(E_x)$, where $E_x = p_x^2/2m^*$, where p_x is x-component of electron's momentum, m^* – transverse effective mass. The search of this function is an only significant

challenge in a way of finding I-V characteristics by original Tsu-Esaki formulation [4] or some of its modifications [1].

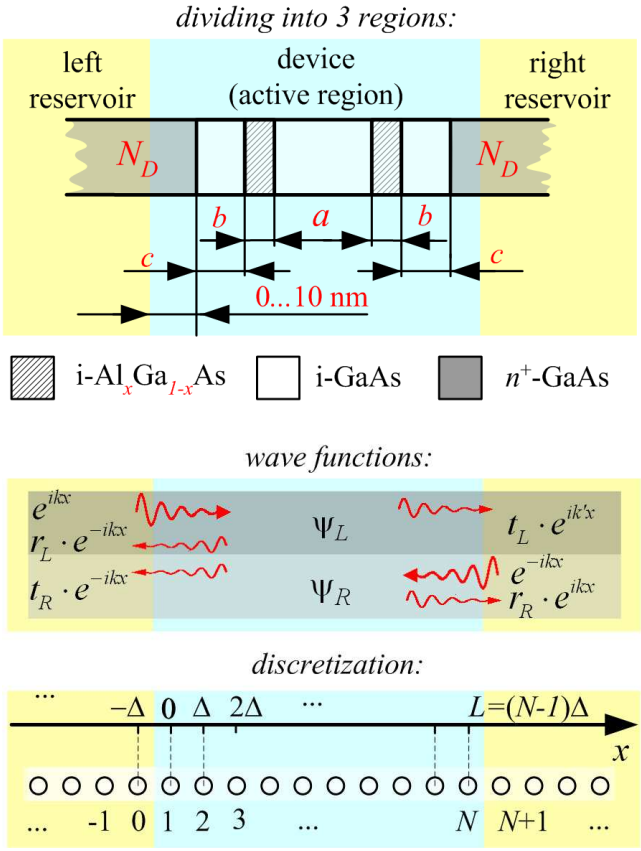

Fig. 1. Model formalization

In order to find, transmission probability for electron that has energy E and move from right (left) reservoir $T(E)$ it is necessary to describe Hamiltonian $\hat{H}$ of the open system that is an active region. Then, implying electron as a spinless particle, $T(E)$ can be found, solving stationary Schrödinger equation

$$\hat{H}\psi = E\psi \tag{1}$$

for envelope function ψ of electron state [5]. Spin is then taken into account by usual way. Potential energy term $U(x)$ in overall Hamiltonian $\hat{H}$ consists of three terms if neglecting exchange-correlation term:

$$\hat{H} = -\frac{\hbar^2}{2}\frac{d}{dx}\frac{1}{m^*(x)}\frac{d}{dx} + U(x) = -\frac{\hbar^2}{2}\frac{d}{dx}\frac{1}{m^*(x)}\frac{d}{dx} + E_C(x) + eV(x) + U_{SCF}(x), \tag{2}$$

where $E_C(x)$ is energy of the bottom of conduction band, $V(x)$ is an applied voltage (it applies such that potential of the right reservoir is enhancing), $U_{SCF}(x)$ is potential energy of electron's interaction with all other electrons, which are considered as a "space charge" (this, in turn, imply that exchange-correlation term is equal to zero).

The last is to be found from Poisson equation:

$$\frac{d}{dx}\left(\varepsilon(x)\frac{dU_{SCF}(x)}{dx}\right) = \frac{e(n(x) - N_D^+(x))}{\varepsilon_0}, \tag{3}$$

where $n(z)$ is electron concentration, $N_D^+(x)$ is a concentration of ionized donor's atoms, $\varepsilon(x)$ is relative dielectric permittivity, ε_0 is dielectric constant.

As electron in the right and left reservoirs are assumed to be spinless quasi-particles being in local equilibrium, each electron individually describes there by the wave-function that is a linear combination of plane waves as it is shown at fig. 1. Therefore, we know the behavior of electrons in reservoirs a priory.

3. MODEL

Modeling procedure consists of the following steps:

1) Search for wave-functions of electron having energy E that arrive to the active region from the ensemble of left/ right reservoir, ψ_L and ψ_R consequently;

2) Search for so-called "partial concentration" of electrons, n_L and n_R in the active region of RTD, using properly normalized electron wave functions. Their sum is equal to total electron concentration in active region n;

3) Solving Poisson equation (3) and equation for $n(x)$ (to be derived below) self-consistently, using $n(x)$ as initial approximation. The results are self-consistent potential $U(x)$ which can be used for finding $T(E)$ by

usual procedure (for example, dividing of active region into piecewise linear regions and applying transfer-matrix formalism [4]);

Then, using $T(x)$ one can calculate current density by Tsu-Esaki formulation.

3.1. Wave functions and ensembles

Behavior of electron at active region with energy close to E depends on from what ensemble it came from: namely from the left or from the right reservoir. This means that state of electron at the active region is mixed [5]. In order to take this into account, wave functions of the electrons, came from both reservoirs ψ_L and ψ_R were found separately for each reservoir. Difference between ψ_L and ψ_R is explained by different "initial conditions": it implies that electron moving from left to right ($k_x > 0$), when searching ψ_L and backward ($k_x < 0$) if vice-versa, when searching ψ_R. In both cases we assume that probability density in incident electron wave is equal to one and there is no reflected wave from the last region (which is right reservoir for ψ_L and left reservoir for ψ_R (fig. 1)).

Using knowledge of wave function in reservoirs, substituting Schrödinger equation in active region by the systems of algebraic equation at the discrete points of structure $x_i = (\Delta - 1)i$ and using general demands for wave function at the boundaries between reservoirs and active region, one can obtain the following finite-difference scheme for ψ_L:

$$\hat{\mathbf{H}}_L \boldsymbol{\psi}_L = \mathbf{C}_L, \tag{4}$$

where:

$$\hat{\mathbf{H}}_L = \begin{bmatrix} 1-\mathrm{i}k_L & 1 & 0 & ... & & & & \\ 1 & c_2 & 1 & 0 & ... & & & \\ 0 & 1 & c_3 & 1 & 0 & ... & & \\ & & \cdot & \cdot & \cdot & & & \\ & & & \cdot & \cdot & \cdot & & \\ & & ... & 0 & 1 & c_{N-2} & 1 & 0 \\ & & & ... & 0 & 1 & c_{N-1} & 1 \\ & & & & ... & 0 & 1 & \mathrm{i}k_R - 1 \end{bmatrix},$$

$\boldsymbol{\psi}_L = [\psi_1, \psi_2, \dots, \psi_N]^{\mathrm{T}}$,

$\mathbf{C}_L = [0,0,...,0]^{\mathrm{T}}$.

Here $k_L = \sqrt{2m^* E}/\hbar$, $k_R = \sqrt{2m^*(E-U_0)}/\hbar$;

$$c_i = \left(\frac{m_i^*/m_{i+1}^* + m_i^*/m_{i-1}^* - 2}{4} + 1 \right) \frac{2m_i^* \Delta^2 (E - U_i)}{\hbar}.$$

Finite-difference scheme for search of ψ_R is:

$$\hat{\mathbf{H}}_R \boldsymbol{\psi}_R = \mathbf{C}_R, \tag{5}$$

where

$$\mathbf{H}_R = \begin{bmatrix} ik_L\Delta - 1 & 1 & 0 & ... & & & & \\ 1 & c_2 & 1 & 0 & ... & & & \\ 0 & 1 & c_3 & 1 & 0 & ... & & \\ & & \cdot & \cdot & \cdot & & & \\ & & & \cdot & \cdot & \cdot & & \\ & & ... & 0 & 1 & c_{N-2} & 1 & 0 \\ & & & ... & 0 & 1 & c_{N-1} & 1 \\ & & & & ... & 0 & 1 & ik_R\Delta - 1 \end{bmatrix},$$

where:

$\boldsymbol{\psi}_R = [\psi_1, \psi_2, \dots, \psi_N]^{\mathrm{T}}$,

$\mathbf{C}_R = [0,0,...,2\mathrm{i}k_R\Delta e^{-ik_R L}]^{\mathrm{T}}$.

These two systems of equations were solved by means of simplified Tomas method [6] as matrixes $\hat{\mathbf{H}}_{R(L)}$ are tridiagonal. Mentioned method is the faster in this case and allows reducing computation time in 200 times compared to the common procedure, which implying matrix inverting.

The results of solving of (4) and (5) are non-normalized wave-function $\tilde{\psi}_L$ and $\tilde{\psi}_L$ that assumed to be related to properly normalized functions so that $\tilde{\psi}_{L(R)} = \sqrt{C_{L(R)}}\,\psi_{L(R)}$, where $C_{L(R)}$ are some constants to be found.

3.2. Partial concentrations

Let's introduce two quantities for active region:

$$g_L(\mathbf{k}, E_x, eV_{act}, x) = \left|\psi_L(E_x, eV_{act}, x)\right|^2 g(\mathbf{k}),$$

$$g_R(\mathbf{k}, E_x, eV_{act}, x) = \left|\psi_R(E_x, eV_{act}, x)\right|^2 g(\mathbf{k}),$$

They will have a physical sense of local density of states of electrons, originated at left (right) reservoir.

Using the conception of local densities of states for calculation of correspondent concentration, one can obtain formulations for partial concentrations n_L and n_R:

$$n_L(x,V_{act}) = \int_0^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} g_L(\mathbf{k},E_x,eV_{act},x) f_{\mathrm{F}}(\mathbf{k},k_{\mathrm{F}}) dk_x dk_y dk_z,$$

$$n_R(x,V_{act}) = \int_{-\infty}^{0}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} g(\mathbf{k},E_x,eV_{act},x) f_{\mathrm{F}}(\mathbf{k},k_{\mathrm{F}}) dk_x dk_y dk_z,$$

where $f_{\mathrm{F}}(\mathbf{k},k_{\mathrm{F}}) = \dfrac{1}{1+\mathrm{e}^{\frac{\frac{\hbar^2}{2m^*}\left(k_x^2+k_y^2+k_z^2\right)-\frac{\hbar^2}{2m^*}k_{\mathrm{F}}^2}{\mathrm{k}T}}}$ is a Fermi function of electrons in reservoirs; V_{act} is net voltage drop at the active region, k_{F} is a Fermi wave vector.

Integration by z and y (it can be performed analytically) and defining of $C_{L(R)}$ will give:

$$n(x,V_{act}) = \frac{N_D^+}{\int_0^{\infty}\frac{1}{\sqrt{E_x}}\ln\left(1+\exp\left(-\frac{E_x-E_{\mathrm{F}}}{\mathrm{k}T}\right)\right)dE_x}\times$$

$$\int_0^{\infty}\left[\frac{1}{\sqrt{E_x}}\left|\tilde{\psi}_L\right|^2\ln\left(1+\exp\left(-\frac{E_x-E_{\mathrm{F}}}{\mathrm{k}T}\right)\right)+\right. \qquad (6)$$

$$\left.\frac{\Theta(E_x-eV_{act})}{\sqrt{E_x-eV_{act}}}\left|\tilde{\psi}_R\right|^2\ln\left(1+\exp\left(-\frac{E_x-E_{\mathrm{F}}-eV_{act}}{\mathrm{k}T}\right)\right)\right]dE_x.$$

Integration in (6) where performed by means of Simpson algorithm, which work with many points x at the same time. It was developed on the basis of standard Matlab procedure "quad", using modifications, which allow working with matrices as input arguments.

3.3. Self-consistent procedure

Finite-differences scheme that corresponds to Poisson equation with boundary conditions of the 2nd type at the active region's boundaries is as follows:

$$U_{i-1}+U_{i+1}-\left(1+\frac{4}{\varepsilon_{i+1}/\varepsilon_i+\varepsilon_{i-1}/\varepsilon_{i+2}+2}\right)U_i = \qquad (7)$$

$$\frac{4\Delta^2}{\varepsilon_0}\frac{n_i-N_i}{(\varepsilon_{i+1}+\varepsilon_{i-1}+2\varepsilon_i)};$$

for all internal points, and for boundaries we assume that $U_1 = U_2$ and $U_{N-1} = U_N$. Here notation N_i was used, which is the same as $N_D^+(x_i)$.

Equation (6) and (7) are being solving self-consistently, using linearized iterative procedure, which is well convergent, if boundary conditions formulated properly [1].

4. RESULTS

The density of electron states at the active region of the simulated RTD under applied voltage 0.05 V and dependence of electron concentration on applied voltage are shown at Fig. 2 and Fig. 3 consequently. The lengths at the fig. 1 are as follows: barriers' thickness $b = 5.6$ nm, well's thickness $a = 5$ nm, spacer's thickness $c = 5$ nm. Donor impurities' concentration in reservoirs $N_D = 10^{23}$ m^{-3}; molar rate of Al in $Al_xGa_{1-x}As$ $x = 0.33$. The following pictures imply that the structure, depicted at Fig. 1 are centered at the point $z = 25$ nm.

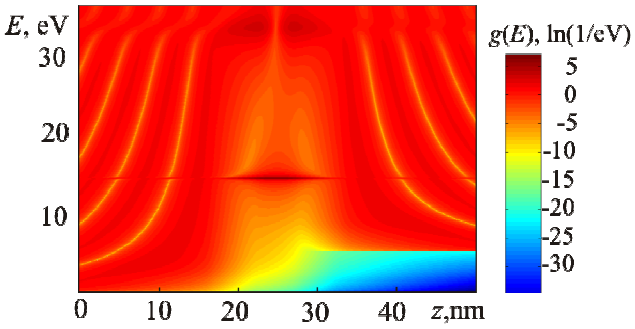

Fig. 2. Density of states g along active region versus transverse electron energy E. Narrow red strip correspondent to metastable energy level.

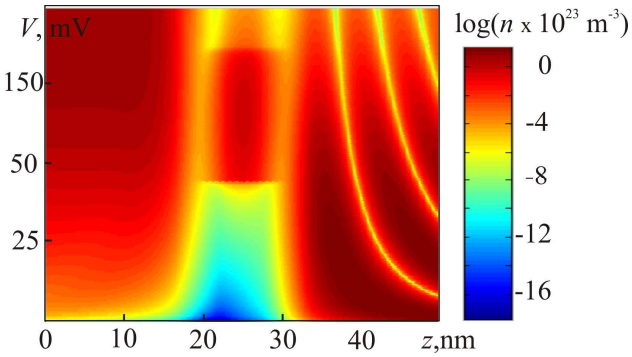

Fig. 3. Dependence of electron concentration *n* along active region on applied voltage. Wide red strip at the center corresponding to charge accumulation at the quantum well.

5. CONCLUSION

Model of RTD's static characteristics were derived from the density functional method and assumption of absence of exchange-correlation term. Simulation procedure was developed, using Matlab. Computational algorithm of simulation procedure was realized in a way that allows reducing computational time and is computationally stable enough.

The further work will be directed at the incorporation of scattering effects into current model and further improvement of visualization as well as computational time further reducing.

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